From force distribution to average coordination number in frictional granular matter

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We study the joint probability distribution of normal and tangential frictional forces in jammed granular media, $P_\mu(f_t, f_n)$, for various friction coefficient μ, especially when $\mu = \infty$. A universal scaling law is found to collapse the data for $\mu = 0$ to ∞ demonstrating a link between force distribution $P_\mu(f_t, f_n)$ and average coordination number, z_c^μ. The results determine z_c^μ for a finite friction coefficient, extending the constraints counting argument of isostatic granular packing to finite frictional packings.

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Granular matter undergos the jamming transition evolving into an amorphous state with a non-zero yield stress as the density increases to a point where all particles are in contact [1]. It has been shown experimentally and numerically that forces are inhomogeneously distributed within a jammed granular system, and further appear to decay exponentially or stretch exponentially for large values of the force [2, 3, 4, 5]. To date, there are various theoretical attempts to describe the force distribution predicting different behavior. For instance, lattice models and like Boltzmann-equation approaches [6] predict an exponential decay. Attempts to fit experimental data within the energy ensemble [7] predict stretched exponential behavior. But the predictions are difficult to justify, since for granular matter energy is neither well defined nor conserved due to frictional forces. An alternative approach is to use the so-called force canonical ensemble with a Boltzmann distribution where the boundary stress, not energy, is the conserved quantity [8, 9, 10]. It is of interest to reduce the above defined force ensemble to obtain a single force distribution, but methods to accomplish this remain in their infancy mainly due to the lack of knowledge on the density of states [9]. A crude approximation would ignore correlations between forces and the contact network as well as the density of states and would predict an exponential decay for the force distribution [8, 9].

Besides the force distribution and the density of states, an additional quantity of interest in this study is the average coordination number, z_c^μ, of a system at the jamming transition with interparticle friction coefficient μ. Despite the importance of z_c^μ for determining the packing stability, there is only one theoretical framework to characterize z_c^μ related to the counting argument of the isostatic conjecture [11]. At the isostatic limit, the configuration of contact forces has a unique solution if the contact network is given, since the number of independent forces is identical to the number of balance equations. Previous works [4, 12, 13, 14, 15, 16, 17] have shown that packings at the jamming transition point are isostatic [12] only for two extreme cases, $\mu = 0$ and $\mu = \infty$, with average coordination number $z_c^0 = 2d$ and $z_c^\infty = d+1$ respectively, where d is the dimension. Recent studies [13] confirm that the indeterminacy of the force ensemble [14] reaches minimum at $\mu = 0$ and ∞.

Lacking more definite theoretical approaches to understand the force distribution, the density of states and z_c^μ for a general μ, we perform a numerical study of the joint force distribution in frictional granular matter, $P_\mu(f_t, f_n)$. Here, the forces at the contacts are normalized by the average forces, in the tangential direction $f_t = \frac{F_t}{\langle F_t \rangle}$ and in the normal direction $f_n = \frac{F_n}{\langle F_n \rangle}$. We show that the key distribution is that of infinite μ, interpreted in terms of the density of states and exponential statistics, providing guidance to theoretical attempts under the statistical framework. We show a universal form of the force ratio distribution $P_\mu(u)$, where u is the ratio of normal and tangential force, $u = \frac{F_t}{F_n}$ valid for all μ, and a scaling law is found to collapse all the $P_\mu(u)$ determining z_c^μ for packings. By using $P_\mu(u)$ we introduce a way to calculate the average coordination number for various μ based on the Maxwell construction of constraint arguments. Thus, we extend the isostatic condition from the limits of $\mu = 0$ and $\mu = \infty$ to finite μ, providing the scaling of z_c^μ, an unsolved nonlinear problem. Our results provide a connection between two important quantities to describe jammed matter: from force distribution to coordination number.

The packings we studied are composed of 10,000 equal size spheres interacting with Hertz forces along the contact direction, F_n, and Mindlin forces in the tangential direction, F_t, plus the Coulomb condition, $F_t \leq \mu F_n$ [15]. We first generate a gas state without friction at an initial volume fraction ϕ_i, then the packing is prepared with friction through a slow compression and relaxation process to achieve equilibrium at a given volume fraction and coordination number as close as possible to the limiting density of the jamming transition. A detailed description of the simulation is given in [17].

We start by constructing an empirical formula of $P_\infty(f_t, f_n)$ based on two numerical results:

(i) We find that the ratio force distribution [3, 4, 15, 16],

$$P_\mu(u) = \kappa \int_0^\infty f_n P_\mu(\kappa u f_n, f_n) df_n, \qquad (1)$$

at infinite friction is characterized by two power-laws

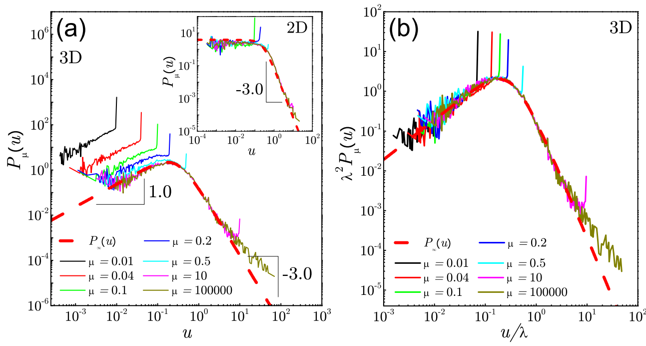

FIG. 1: (a) and the inset are log-log plots of the PDF of u respectively in 3D and 2D for various μ; (b) Log-log plot of the collapsed $P_\mu(u)$ for various μ in 3D. The red dash-lines both in (a) and (b) are plots of $P_\infty(u) = \frac{\kappa(d-1)}{(1+\kappa^2 u^2)^{3/2}} (\frac{\kappa u}{\sqrt{1+\kappa^2 u^2}})^{d-2}$, where we use $\kappa = 3.80$ and 3.43 respectively for 2D and 3D from a direct measurement of the simulation;

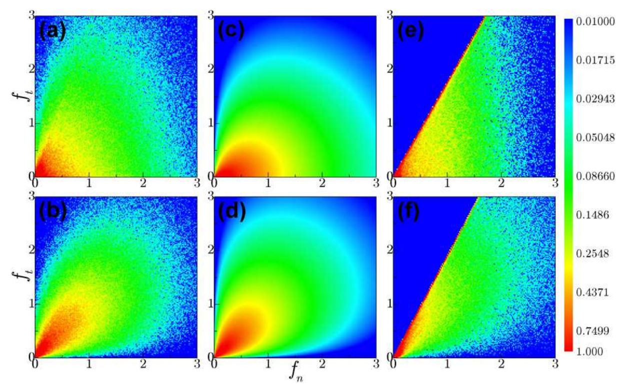

FIG. 2: (a), (b) Contour plotting of $P_\infty(f_t, f_n)$ from simulation results in 2D and 3D respectively; (c), (d) Contour plotting of the empirical formula Eq. (2) with $a = 0.8$ in 2D and 3D respectively; (e), (f) Contour plotting of $P_{0.3}(f_t, f_n)$ from simulation result in 2D and 3D respectively with $\mu = 0.3$. In (a), (b), (e) and (f), we superpose the data from 20 individual configurations, each of them contains 10,000 grains.

with exponents equal to 0 and -3 in 2D, and 1 and -3 in 3D respectively at $u \to 0$ and $u \to \infty$, where $\kappa = \frac{\langle F_n \rangle}{\langle F_t \rangle}$, is an anisotropy parameter. Figure 1a plots $P_\mu(u)$ for various values of μ, showing that all $P_\mu(u)$ displays similar behavior having two power-law slopes except for a sharp peak at $u = \mu$, due to sliding contacts reaching the Coulomb threshold. A correct form of force distribution should predict this power-law behavior.

Notice that previous 2D simulations [3, 16] have reported a plateau of $P_\mu(u)$ in the region of $[0, \mu]$, corresponding to the first power-law of $P_\mu(u)$ with the exponent equal to 0, shown in the inset of Fig. 1a. The second power-laws only appears for very large values of μ and has not been reported by previous studies. We only show $P_\mu(u)$ with $\mu > 0.1$ for 2D in the inset of Fig. 1a due to the difficulty of preparing disordered 2D monodisperse packing at small values of μ.

(ii) We find that the contour plot of $P_\infty(f_t, f_n)$ follows the geometric behavior shown in Fig. 2a and 2b, especially in 3D case where $P_\infty(f_t, f_n)$ is symmetric in the space of (f_t, f_n). We will show later on that this symmetric behavior only occurs at large enough forces in 3D. A correct form of the force distribution should predict this behavior.

By fitting our numerical data, we find an empirical form of $P_\infty(f_t, f_n)$ for infinite friction, consistent with (i) and (ii). We describe it by defining new variables $f = \sqrt{f_t^2 + f_n^2}$ and $\theta = \arctan(\frac{f_t}{f_n})$,

$$P_\infty(f, \theta) = a\ g(\theta)\ e^{-\sqrt{a} f}, \tag{2}$$

where a is a constant, which could be regarded as the inverse of the angoricity [8, 9, 10]. By fitting this distribution we find

$$g(\theta) = (d-1)(\sin\theta)^{d-2}\cos\theta,$$

which can be regarded as the density of states approximately for the force ensemble at $\mu = \infty$. Equation (2), plotted in Fig. 2c and 2d, shows similar pattern to the simulation results of Fig. 2a and 2b. We further study the contour plot of $P_\mu(f_t, f_n)$ at $\mu = 0.3$ shown in Fig. 2e and 2f. $P_{0.3}(f_t, f_n)$ displays the same pattern inside the Coulomb cone as when $\mu = \infty$. We therefore suggest that the study of force distribution for frictional packing should focus on packings with $\mu = \infty$. The density of state $g(\theta)$ describes the probability of the contact forces for a single contact to have an angle θ [we note that there is no obvious geometric meaning for θ, which is not the angle between the normal and the net contact force: $\theta = \arctan(\frac{f_t}{f_n}) = \arctan(\kappa\frac{F_t}{F_t}) \neq \arctan(\frac{F_t}{F_t})$] and indicates that normal and tangential forces are correlated to each other even when there is no Coulomb constraint.

We define $P_<(\theta)$ as the cumulative probability distribution of θ indicating the probability of the contact forces for a single contact to have an angle less than θ, such that $g(\theta) = \frac{dP_<(\theta)}{d\theta}$. We find:

$$P_<(\theta) = (\sin\theta)^{d-1}. \tag{3}$$

This simple form $P_<$ could lead to a theoretical approach to the force distribution since it provides the density of states within the statistical mechanics framework [9, 10].

Equation (2) implies that $P_\infty(f, \theta)/g(\theta) = ae^{-\sqrt{a} f}$ is independent of θ. We plot $P_\infty(f, \theta)/g(\theta)$ for various values of θ in Fig. 3a to further compare with the simulation results. We find that all the curves collapse with exponential tails in the region of $f > 1$, indicating that the empirical form of Eq. (2) captures the main features of the force distribution for large forces. $P_\infty(f, \theta)/g(\theta)$ has a peak at $f \simeq 1$ when θ is small, and exhibits a monotonic exponential decrease when θ is close to $\frac{\pi}{2}$. This implies that the probabilities of single forces, $P_\infty(f_n)$ and $P_\infty(f_t)$, have different behavior as shown in Fig. 3b: $P_\infty(f_n)$ displays a peak at $f \simeq 1$ while $P_\infty(f_t)$ does not.

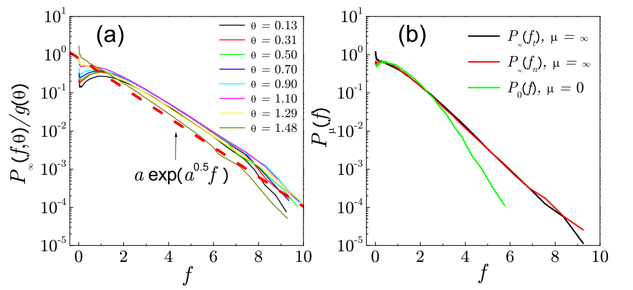

FIG. 3: (a) Log-linear plot of $P_\infty(f,\theta)/g(\theta)$ for various value of θ in 3D. All the curves well collapse with a pure exponential tail in the region of $f > 1$. The red dashed-line is function of $ae^{-\sqrt{a}f}$ with $a = 0.8$. (b) Log-linear plot of $P_\infty(f_t)$, $P_\infty(f_n)$ and $P_0(f_n)$.

This result is consistent with previous experimental studies of frictional packings [18]. In Fig. 3b we plot the force distribution at $\mu = 0$ and compare with $\mu = \infty$. We conclude that $P_0(f_n)$ has a stretched exponential tail close to Gaussian with a exponent $\beta = 1.65$ due to local entropy maximization [19].

By using Eq. (1) and Eq. (2) we obtain a ratio force distribution $P_\infty(u)$, shown in Fig. 1, as a red dashed-line in good agreement with numerical results. This result further confirms that our empirical formula Eq. (2) is reasonable.

Further, we show that the ratio distribution is the link between the ensemble of forces and the average coordination number. We find that $P_\mu(u)$ can be rescaled to a single curve (except for the peak at μ), with scaling factors equal to λ and λ^2, for the y and x axes, respectively. We find $\lambda = 1$ in 2D and $\lambda = (z_c^0 - z_c^\infty)/(z_c^0 - z_c^\mu)$ in 3D, as plotted in Fig. 1b. In the 2D case, $P_\mu(u)$ collapses without scaling, so $\lambda = 1$. The 3D case is different, where we find that $\lambda \to 1$ when $\mu \to \infty$, so $P_\infty(u)$ does not change after multiplying the scaling factors. The factor λ diverges at $\mu = 0$, implying that $P_\mu(u)$ reduces to a delta function at $\mu = 0$ due to the fact that all contact forces reach the Coulomb threshold in a pure frictionless packing.

Next, we show that the universal form of $P_\infty(u)$ determines z_c^μ for any μ, hereby extending the isostatic counting argument from $\mu = 0$ and $\mu = \infty$ to finite values of μ. From linear counting arguments we know that $z_c^0 = 2d$ and $z_c^\infty = d+1$, and we want to interpolate to finite μ and obtain z_c^μ. Below, we show that the Maxwell constraint arguments based on the number of redundant constraints provides the framework to derive z_c^μ. Analysis of the coordination number of granular packings can be related to the Maxwell constraints counting in the rigidity percolation theory [20]:

$$F = \frac{zd}{2}N - N_c + N_r, \tag{4}$$

where F is the number of degrees of freedom (or floppy modes) satisfying $F \geq 0$, N is the number of grains, N_c is the number of constraints, N_r is the number of redundant constraints, and z is the coordination number. At the jamming transition, $F = 0$, resulting in a minimum value of z, i.e., z_c^μ. Here $zdN/2$ is equal to the total number of unknown force variables for a fixed force network.

We consider a static packing with both force and torque balances, but without any typical constraints of translation and rotation. For packings with $\mu = \infty$, the number of constraint N_c will be equal to the number of force balance equation, dN, plus the number of torque balance equation, $d(d-1)N/2$, i.e., $N_c(\infty) = d(d+1)N/2$. There exists reasonable evidence [1, 4, 11, 12, 13, 14, 15, 16, 17] to believe that at the jamming transition, $N_r(\infty) = 0$, implying a conjecture that the Maxwell counting approximation is exact. Therefore, $z = z_c^\infty = d + 1$. Another important case is at $\mu = 0$. Here the redundant constraints, $N_r(0) = d(d-1)N/2$, is equal to the number of torque balance equation due to the absence of tangential force. Further, we must add $z(d-1)N/2$ extra constraints to $N_c(0)$, corresponding to equations of tangential force equal to zero, ${F_t}^i = 0$. Therefore, $N_c(0) = N_c(\infty) + z(d-1)N/2$ and we obtain $z = z_c^0 = 2d$.

Analyzing intermediate values of μ, is complicated since many inequality constrains are created as $\mu {F_n}^i - {F_t}^i \geq 0$. Calculating z_c^μ becomes a nonlinear problem and can be understood as an optimization of an outcome based on some set of constraints, i.e., minimizing a Hamiltonian of the system, $\mathbb{H}(\mathbf{F_n}, \mathbf{F_t})$, over a convex polyhedron specified by linear and non-negativity constraints. An interesting feature found in previous studies is that z_c^μ monotonically decreases from $2d$ to $d+1$ with increasing μ [4, 13, 16, 17], implying that we can map this non-linear problem to a linear one by considering a monotonic change in the number of constraints in Eq. (4) with increasing μ.

The above analysis suggests to extend the Maxwell counting argument Eq. (4) to a system with finite μ as:

$$F = \frac{z_c^\mu d}{2}N - N_c(\infty) + [N_r(0) - z_c^\mu(d-1)N/2]\,\eta(\mu) = 0, \tag{5}$$

where $\eta(\mu)$ is an undetermined monotonic function ranging from 1 to 0 as μ ranges from 0 to ∞. The problem is reduced to choosing a functional form for $\eta(\mu)$.

To determine $\eta(\mu)$, we notice that it should be related to the sliding rate of packings, i.e., the ratio of the number of the sliding contacts to the number of total contacts in a packing, denoted $S(\mu)$. By definition, $S(\mu)$ is determined by $P_\mu(u)$, providing a link between coordination number an force distribution:

$$S(\mu) = 1 - \int_0^\mu P_\mu(u)du = 1 - \int_0^\mu \lambda^2 P_\infty(\lambda u)du \tag{6}$$

The limiting cases are $S(0) = 1$ and $S(\infty) = 0$, and $S(\mu)$ has the same monotonic behaviour as $\eta(\mu)$.

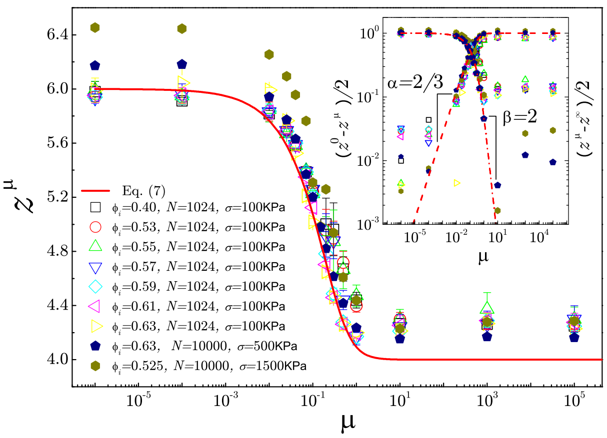

FIG. 4: z^μ versus μ for various initial volume fraction ϕ_i in 3D. The red solid line is the theory result predicted by Eq. (7). In the inset, the red-dash and dash-dot lines are the prediction of $(z^0 - z^\mu)/2$ and $(z^\mu - z^\infty)/2$, respectively, in comparison with simulations.

While $\eta(\mu)$ must be a function of $S(\mu)$, there are many choices for the functional relation between both quantities. We determine this functional form by fitting the simulations. Setting $\eta(\mu) = 1 - (1 - S(\mu))/\lambda$ provides very good fitting of z_c^μ with simulations both in 2D and 3D. Substituting $\eta(\mu)$ into Eq. (5), we arrive at a cubic equation for z_c^μ in 3D:

$$\frac{1}{\kappa^2\mu^2}\left(\frac{6 - z_c^\mu}{2}\right)^3 + 3\left(\frac{6 - z_c^\mu}{2}\right) - 3 = 0. \tag{7}$$

It can be shown that Eq. (7) predicts two power-law relations, $z_c^0 - z_c^\mu \sim \mu^\alpha$, and $z_c^\mu - z_c^\infty \sim \mu^{-\beta}$, respectively for $\mu \to 0$ and $\mu \to \infty$, where $\alpha = 2/3$ and $\beta = 2$. In Fig. 4 we plot z_c^μ obtained from the cubic Eq. (7) and compare with simulation data in 3D. The asymptotic predictions of $\alpha = 2/3$ and $\beta = 2$ are in good agreement with simulation results shown in the inset of Fig. 4. It is difficult to check the value of β due to the difficulty of preparing a 3D packing as close as possible to $z_c^\infty = 4$. To solve this problem, we prepare larger packings slightly above the critical point with a small constant pressure, and z_c^μ is replaced by z^μ without suffix. This result is shown in Fig. 4 with two sets of data for pressure $\sigma =$ 500Kpa and $\sigma = 1500$KPa. We can see that the power law of coordination number is independent of pressure even when z^μ is far from the isostatic value.

When we combine power-law finding of z_c^μ with our theoretical work of [17] in 3D, where z_c^μ is linked to the volume fraction ϕ_c^μ with a simple formula, $\phi_c^\mu = z_c^\mu/(z_c^\mu + 2\sqrt{3})$, then we solve the relation between ϕ_c^μ, z_c^μ and μ; ϕ_c^μ follows the same scaling behavior with μ, $\phi_c^0 - \phi_c^\mu \sim \mu^\alpha$, and $\phi_c^\mu - \phi_c^\infty \sim \mu^{-\beta}$. Recent experiments [21] in 3D investigate the preparation of packings close to the random loose packing limit. They find $\alpha = 0.51 \pm 0.25$ and $\beta = 0.89 \pm 0.16$. Their measurement of β is far away from our prediction which could be due to the same reason as us, i.e., the difficulty of preparing packing as close as possible to $z_c^\infty = 4$.

In the 2D case, $\eta(\mu) = S(\mu)$ since $\lambda = 1$, and we have

$$z_c^\mu = \left[4 + \frac{2\kappa\mu}{(1+\kappa^2\mu^2)^{1/2}}\right] / \left[1 + \frac{\kappa\mu}{(1+\kappa^2\mu^2)^{1/2}}\right]. \tag{8}$$

This equation predicts $\alpha = 1$ and $\beta = 2$, close to our simulation result of $\beta = 1.86$. We can not determine the value of α from simulation due to the difficulty of preparing disordered 2D monodisperse packings for small values of μ, and the polydispersity of packings may slightly affect these two indices. Previous simulations [16] of polydisperse 2D packings have $\alpha = 0.7$, still close to our predictions.

In summary, we develop a framework to study the connection between the force distribution and the coordination number. Some aspects of this connection remain empirical, including the density of states, $g(\theta)$, and the scaling factor λ, allowing for the collapse of $P_\mu(u)$ into a single curve. Overall, the obtained mathematical forms of the density of states, the different force distributions, the coordination number and volume fraction, may allow for their incorporation into a statistical force ensemble of jammed matter [9, 10]. This may facilitate the solution of outstanding open problems such as the prediction of the power law scaling of the pressure, the coordination number and elastic moduli with the volume fraction near the jamming transition [1].

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